Gauge Variant Symmetries for the Schrödinger Equation

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Abstract

The last multiplier of Jacobi provides a route for the determination of families of Lagrangians for a given system. We show that the members of a family are equivalent in that they differ by a total time derivative. We derive the Schrödinger equation for a one-degree-of-freedom system with a constant multiplier. In the sequel we consider the particular example of the simple harmonic oscillator. In the case of the general equation for the simple harmonic oscillator which contains an arbitrary function we show that all Schrödinger equations possess the same number of Lie point symmetries with the same algebra. From the symmetries we construct the solutions of the Schrödinger equation and find that they differ only by a phase determined by the gauge.

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1 Introduction

Jacobi's Last Multiplier is a solution of the linear partial differential equation [4, 12],

$$\frac{\partial M}{\partial t} + \sum_{i=1}^{N} \frac{\partial (M a_i)}{\partial x_i} = 0, \tag{1}$$

where $\partial_t + \sum_{i=1}^{N} a_i \partial_{x_i}$ is the vector field of the set of first-order ordinary differential equations for the N dependent variables x_i. The relationship between the Jacobi Last Multiplier and the Lagrangian, *videlicet* [4, 12]

$$\frac{\partial^2 L}{\partial \dot{x}^2} = M \tag{2}$$

for a one-degree-of-freedom system, is perhaps not widely known although it is certainly not unknown as can be seen from the bibliography in [9]. If two multipliers, M_1 and M_2, are known, their ratio is a first integral. In the case of a conservative system with the standard energy integral

$$E = \tfrac{1}{2}\dot{x}^2 + V(x) \tag{3}$$

and Lagrangian

$$L = \tfrac{1}{2}\dot{x}^2 - V(x) \tag{4}$$

it is evident from (2) that one multiplier is a constant – taken to be 1 without loss of generality – and so all multipliers are first integrals. This combined with (2) is a simple recipe for the generation of a Lagrangian. One has

$$\frac{\partial^2 L}{\partial \dot{x}^2} = 1 \quad \Longrightarrow \quad L = \tfrac{1}{2}\dot{x}^2 + \dot{x} f_1(t,x) + f_2(t,x), \tag{5}$$

where f_1 and f_2 are arbitrary functions of integration. Naturally different multipliers give rise to different Lagrangians. For a study of these in the classical context with particular reference to their inequivalence and Noether symmetries see [11]. Lagrange's equation of motion for (5) is

$$\ddot{x} + \frac{\partial f_1}{\partial t} - \frac{\partial f_2}{\partial x} = 0 \tag{6}$$

whereas that for (4) is

$$\ddot{x} + V'(x) = 0 \tag{7}$$

so that the requirement that the two Newtonian equations be the same is

$$\frac{\partial f_1}{\partial t} - \frac{\partial f_2}{\partial x} = V'(x) \tag{8}$$

which is a constraint on the doubly infinite family of functions, f_1 and f_2. This constraint may be expressed through setting

$$f_1 = \frac{\partial g}{\partial x}, \quad f_2 = \frac{\partial g}{\partial t} - V(x), \tag{9}$$

where $g(t,x)$ is an arbitrary function of its arguments. Consequently the Lagrangian, (5), becomes

$$\begin{aligned} L &= \tfrac{1}{2}\dot{x}^2 - V(x) + \dot{x}\frac{\partial g}{\partial x} + \frac{\partial g}{\partial t} \\ &= \tfrac{1}{2}\dot{x}^2 - V(x) + \dot{g}, \end{aligned} \tag{10}$$

ie, the functions f_1 and f_2 are a consequence of the arbitrariness of a Lagrangian with respect to a total time derivative, the gauge function.

Although we confine our attention to equations of motion such as (7) with a constant multiplier, the discussion above is quite general. By way of example consider the Hamiltonian [3] [ex 18, p 433]

$$H = \tfrac{1}{2}\left(\frac{1}{q^2} + p^2 q^4\right) \tag{11}$$

with Lagrangian and equation of motion

$$L = \tfrac{1}{2}\left(\frac{\dot{q}^2}{q^4} - \frac{1}{q^2}\right) \qquad q\ddot{q} - 2\dot{q}^2 - q^2 = 0. \tag{12}$$

From the Lagrangian and (2) it is evident that a multiplier is

$$M = \frac{1}{q^4} \tag{13}$$

and so the general Lagrangian is

$$L = \tfrac{1}{2}\frac{\dot{q}^2}{q^4} + \dot{q}f_1(t,q) + f_2(t,q). \tag{14}$$

The precise equation of motion in (12) is obtained if f_1 and f_2 are constrained according to

$$\frac{\partial f_1}{\partial t} - \frac{\partial f_2}{\partial q} = -\frac{1}{q^3}. \tag{15}$$

If we write

$$f_1 = \frac{\partial g}{\partial x} \quad \text{and} \quad f_2 = -\frac{\partial g}{\partial t} - \frac{1}{2q^2}, \tag{16}$$

we clearly see that the imposition of the constraint (15) again introduces an arbitrary gauge. We note that the Hamiltonian, (11), is connected by a canonical transformation, specifically $Q = -q^{-1}$, $P = q^2 p$ yields $K = \frac{1}{2}\left(P^2 + Q^2\right)$, to the standard Hamiltonian of the simple harmonic oscillator.

Naturally we do not have to confine our attention to linear problems. For example the simple pendulum with Newtonian equation of motion

$$\ddot{q} + \omega^2 \sin q = 0 \tag{17}$$

has a Lagrangian of the form given in (5), but now the constraint on the functions f_1 and f_2 is

$$\frac{\partial f_1}{\partial t} - \frac{\partial f_2}{\partial q} = \omega^2 \sin q \tag{18}$$

which can be satisfied if we introduce a gauge function, $g(t, q)$, such that

$$f_1 = \frac{\partial g}{\partial q} \quad \text{and} \quad f_2 = \frac{\partial g}{\partial t} - \omega^2 \left(1 - \cos q\right). \tag{19}$$

In this paper we wish to explore the implications of generality of the Lagrangian, (5), in the context of the corresponding Schrödinger Equation. To make the work quite explicit we use the simple harmonic oscillator as a vehicle. There is a simple reason for this choice. The simple harmonic oscillator is richly endowed with symmetry which are the eight Lie point symmetries of its Newtonian equation of motion, the five Noether point symmetries of its Action Integral and the five plus one plus infinity Lie point symmetries of its Schrödinger Equation. The last provide an algorithmic route to the determination of the wave-functions [5, 1, 10, 2]. What we find here is that the Schrödinger Equation of the Hamiltonian corresponding to the Lagrangian with an arbitrary gauge function has the same number of Lie point symmetries as the standard Schrödinger Equation for the simple harmonic oscillator.

However, the unknown functions, f_1 and f_2 are present in the symmetries. Nevertheless the determination of the wave-functions using these Lie point symmetries proceeds without hindrance.

2 Schrödinger Equation

The canonical momentum for (5) is

$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x} + f_1 \tag{20}$$

so that

$$\begin{aligned} H &= p\dot{x} - L \\ &= \tfrac{1}{2}p^2 - pf_1 + \tfrac{1}{2}f_1^2 - f_2 \end{aligned} \tag{21}$$

is the Hamiltonian. Whether one uses the Weyl quantisation formula or the symmetrisation of pf_1 make no difference to the form of the Schrödinger Equation corresponding to (21) which is

$$2i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} + 2if_1\frac{\partial u}{\partial x} + \left(f_1^2 - 2f_2 + i\frac{\partial f_1}{\partial x}\right)u. \tag{22}$$

The Schrödinger Equation, (22), is quite general. We now introduce the simple harmonic oscillator with Newtonian equation of motion $\ddot{x} + k^2x = 0$ so that the constraint (8) is

$$\frac{\partial f_1}{\partial t} - \frac{\partial f_2}{\partial x} = k^2x. \tag{23}$$

One notes that neither of the derivatives in the constraint appears in the Schrödinger Equation, (22). As we observed above, the reason for using the simple harmonic oscillator as the explicit example is simply due to its generous supply of point symmetries.

The Lie point symmetries of (22) subject to the constraint (23) are[1]

$$
\begin{aligned}
\Gamma_1 &= \cos(kt)\,\partial_x + [\cos(kt) f_1 - \sin(kt)kx]\, iu\,\partial_u \\
\Gamma_2 &= -\sin(kt)\,\partial_x - [\sin(kt) f_1 + \cos(kt)kx]\, iu\,\partial_u \\
\Gamma_3 &= \partial_t + \left(f_2 + \frac{1}{2}\,k^2x^2\right) iu\,\partial_u \\
\Gamma_4 &= \cos(2kt)\,\partial_t - \sin(2kt)kx\,\partial_x \\
&\quad + \left[i\cos(2kt)\left(f_2 - \frac{1}{2}\,k^2x^2\right) - k\sin(2kt)\left(ixf_1 - \frac{1}{2}\right)\right] u\partial_u \\
\Gamma_5 &= -\sin(2kt)\partial_t - \cos(2kt)kx\partial_x \\
&\quad - \left[i\sin(2kt)\left(f_2 - \frac{1}{2}\,k^2x^2\right) + k\cos(2kt)\left(ixf_1 - \frac{1}{2}\right)\right] u\partial_u \\
\Gamma_6 &= u\,\partial_u \\
\Gamma_7 &= s(t,x)\partial_u, \qquad (24)
\end{aligned}
$$

where $s(t,x)$ is a solution of (22), which is a representation of the well-known algebra, $\{sl(2,R) \oplus_s W\} \oplus_s \infty A_1$, of the Schrödinger Equation for the one-dimensional linear oscillator and related systems. The presence of the functions f_1 and f_2 subject to the constraint (23) does not affect the number of Lie point symmetries of (22) vis-à-vis the number for the Schrödinger Equation for the simple harmonic oscillator[2]. The symmetries listed in (24) reduce to those for the standard Schrödinger Equation of the simple harmonic oscillator if one sets, say, $f_1 = 0$ and $f_2 = -\frac{1}{2}k^2x^2$, which is an obvious solution of (23).

3 Creation and Annihilation Operators

For the purposes of quantum mechanics one usually writes symmetries of the structure of Γ_1 and Γ_2 and Γ_4 and Γ_5 in terms of an exponential rather than

[1] Thanks to Nucci's interactive package for the computation of Lie symmetries [7, 8].

[2] Although we make no attempt to prove it, one can easily believe that the result is independent of the particular potential. It is just that the Schrödinger Equation with a general potential is rather lacking in Lie point symmetries apart from Γ_6 and Γ_7. We emphasise, however, that it is not invariably the case that the Schrödinger Equation constructed from a given Hamiltonian has the same number of Lie point symmetries as the corresponding Lagrangian has Noether point symmetries plus Γ_6 and Γ_7 which are a consequence of the linearity of the equation.

trigonometric functions. Thus we write

$$
\begin{aligned}
\Gamma_{1\pm} &= \exp[\pm kit]\{\partial_x + i(f_1 \pm ikx)u\partial_u\} && (25)\\
\Gamma_{4\pm} &= \exp[\pm 2kit]\left\{\partial_t \pm kix\partial_x + i\left[\left(f_2 - \tfrac{1}{2}k^2x^2\right) \pm k\left(2if_1 - \tfrac{1}{2}\right)\right]u\partial_u\right\}. && (26)
\end{aligned}
$$

The normal route to the solution of the Schrödinger Equation, (22), is to use the symmetries (25)[3] which are the time-dependent progenitors of the well-known creation and annihilation operators of Dirac in the case that f_1 and f_2 are restricted as above.

To solve the Schrödinger Equation, (22), using Lie's method we reduce (22) to an ordinary differential equation by using the invariants of the symmetries as a source of the variables. We must also be cognisant of the need for the solution of (22) to satisfy the boundary conditions at $\pm\infty$. With this requirement in mind we take Γ_{1+}. The associated Lagrange's system is

$$\frac{\mathrm{d}t}{0} = \frac{\mathrm{d}x}{1} = \frac{\mathrm{d}u}{i\left(f_1 + kix\right)u} \tag{27}$$

which gives the characteristics t and $u\exp\left[\frac{1}{2}kx^2 - ig(t,x)\right]$, where we have made use of the first of (9) and the fact that t is a characteristic. To find the solution corresponding to Γ_{1+} we write

$$u(t,x) = h(t)\exp\left[-\tfrac{1}{2}kx^2 + ig(t,x)\right], \tag{28}$$

where $h(t)$ is to be determined, and substitute it into (22) which simplifies to

$$i\dot{h} = \tfrac{1}{2}kh$$

so that

$$h(t) = \exp\left[-\tfrac{1}{2}kit\right]$$

and

$$u(t,x) = \exp\left[-\tfrac{1}{2}kit - \tfrac{1}{2}kx^2 + ig(t,x)\right] \tag{29}$$

up to a normalisation constant which we ignore. With $g = 0$ we recognise the ground-state solution for the time-dependent Schrödinger Equation of the simple harmonic oscillator.

[3]These are, as equally Γ_1 and Γ_2, often termed 'solution symmetries' since they correspond to the solutions of the corresponding Newtonian equation of motion. For the Schrödinger Equation the symmetries Γ_7 are *the* solution symmetries, but they do not play the same role as Γ_1 and Γ_2 or $\Gamma_{1\pm}$ which is the specification of the potential.

Evidently we use Γ_{1-} as a time-dependent 'creation operator'. If we write the left hand side of (29) as u_0, we can have a solution symmetry of the form

$$\Gamma_{70} = u_0(t,x)\partial_u, \tag{30}$$

where the subscript, 7j, means that we are using the symmetry Γ_7 with the specific solution, $u_j(t,x)$. We use the closure of the Lie algebra under the operation of taking the Lie Bracket to obtain further solutions. Thus

$$[\Gamma_{1-},\, \Gamma_{70}]_{LB} = \left\{-kx + i\frac{\partial g}{\partial x} - (if_1 + kx)\right\} \exp\left[-\tfrac{3}{2}kit - \tfrac{1}{2}kx^2 + ig\right]\partial_u \tag{31}$$

so that we have

$$u_1(t,x) = -2kx \exp\left[-\tfrac{3}{2}kit - \tfrac{1}{2}kx^2 + ig\right]. \tag{32}$$

Likewise $[\Gamma_{1-},\, \Gamma_{71}]_{LB}$ gives

$$u_2(t,x) = \left(4k^2x^2 - 2k\right) \exp\left[-\tfrac{3}{2}kit - \tfrac{1}{2}kx^2 + ig\right]. \tag{33}$$

On the other hand the Lie Bracket of Γ_{4-} with Γ_{70} gives

$$\tilde{u}_2(t,x) = \left(-ik + 2ik^2x^2\right) \exp\left[-\tfrac{3}{2}kit - \tfrac{1}{2}kx^2 + ig\right], \tag{34}$$

which is u_2 up to a constant factor, *ie* Γ_{4-} acts as a double creation operator. One is not surprised that Γ_{4+} is a double annihilation operator. Obviously Γ_{1+}, since it was used to derive the ground state, is the annihilation operator.

Finally the Lie Bracket of $i\Gamma_3$ with Γ_7 yields the energy. For example with Γ_{72} one has

$$[i\Gamma_3,\, \Gamma_{72}]_{LB} = \tfrac{5}{2}ku_2\partial_u. \tag{35}$$

In general the action of Γ_{1-} on a solution symmetry Γ_{7j}, which has been generated by the j-fold action of Γ_{1-} on Γ_{70} by means of the taking of the Lie Bracket, is

$$[\Gamma_{1-},\, \Gamma_{7j}]_{LB} = \Gamma_{7,,j+1}$$

and the energy eigenvalue is given by the action of $i\Gamma_3$ as

$$\begin{aligned} [\Gamma_3,\, \Gamma_{7j}]_{LB} &= (j+\tfrac{1}{2})ku_j\partial_u \\ &= (j+\tfrac{1}{2})\Gamma_{7,,j}. \end{aligned}$$

It should be quite evident that the operators $\Gamma_{1\pm}$ are the sources of the creation and annihilation operators introduced by Dirac for the time-independent Schrödinger equation of the simple harmonic oscillator. Similar operators are found for time-dependent quadratic Hamiltonians and these play roles similar to those played by the operators reported here.

4 Discussion

If one derives a Jacobi Last Multiplier for a one-degree-of-freedom system, the connection, (2), between the multiplier and the Lagrangians leads to a doubly infinite family of Lagrangian for the same multiplier and so a doubly infinite family of Lagrangian equations of motion. Insistence that the Lagrangians be specific to the given Newtonian equation of motion still leaves an infinite class of Lagrangians related by a gauge function.

In the case of a constant multiplier one obtains a Lagrangian quadratic in the velocity and hence an Hamiltonian quadratic in the momentum. From the Hamiltonian one can construct a Schrödinger Equation of quite general form. To enable the obtaining of precise results we specialised to the simple harmonic oscillator. We found that the number of Lie point symmetries of the Schrödinger Equation was unchanged from that of the standard Schrödinger Equation for the simple harmonic oscillator. The algebra is the same even with the presence of f_1 and f_2 subject to the single constraint (23). Using the exceptional Lie point symmetries in the combinations, $\Gamma_{1\pm}$, $\Gamma_{4\pm}$ and Γ_3, we were able to construct solutions for the Schrödinger Equation and found that these Lie point symmetries acted as creation, annihilation and energy operators.

Classically the presence of the gauge function does not affect the form of the Lagrangian equation of motion. In the case of the simple harmonic oscillator we saw that the wave functions and energy levels are the same as when the usual Schrödinger Equation for the simple harmonic oscillator is used with the exception of a phase, $\exp[ig(t,x)]$, which otherwise does not intrude.

It is a natural question to enquire of the extension of the considerations

in this paper to the Hamiltonians of the form

$$H = \tfrac{1}{2}p^2 + V(q,t) \quad \Leftrightarrow \quad L = \tfrac{1}{2}\dot{q}^2 - V(q,t) \tag{36}$$

for which the Jacobi Last Multiplier is also 1 as calculated by means of a reversal of (2). In the case that V is quadratic in q the results reported here persist *mutatis mutandis* since there is no change in the underlying basis of symmetry [2]. For a general potential as in (36) there is a constant multiplier which means that any other multiplier is an integral. However, the calculation of additional multipliers is either by the solution of (1) or the method of Lie using the symmetries of the Schrödinger equation. Neither method is fruitful for a general $V(t,q)$. The relationship between a Jacobi Last Multiplier and a Lagrangian is quite specific. A Lagrangian obtained from a Jacobi Last Multiplier and consistent with the equations of motion is under no obligation to possess a sufficient number of first integrals for the Theorem of Liouville to apply. The absence of symmetry in the Euler-Lagrange equation means an absence of Jacobi Last Multipliers apart from the one which generates (36) (in this case). Consequently there is an absence of integrals. The one multiplier gives the Lagrangian. The absence of others denies integrability.

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